

Available online at www.sciencedirect.com



Chemical Physics Letters 390 (2004) 522-530

CHEMICAL PHYSICS LETTERS

www.elsevier.com/locate/cplett

Author Index to Volume 390

Abdoul-Carime, H. and E. Illenberger, Degradation of vitamin C by low-energy electron	is 390 (2004) 481
Achiba, Y., see Gloter, A.	390 (2004) 462
Adler, J., see Prawer, S.	390 (2004) 458
Ahn, DS., S. Lee and B. Kim, Solvent-mediated tautomerization of purine: single to que proton transfer	adruple 390 (2004) 384
Akimoto, S., I. Yamazaki, A. Murakami, S. Takaichi and M. Mimuro, Ultrafast ex relaxation dynamics and energy transfer in the siphonaxanthin-containing green alga	citation
fragile	390 (2004) 45
Al-Kahali, M.H.S.N., see Ridley, T.	390 (2004) 376
Aliat, A., E.V. Kustova and A. Chikhaoui, State-to-state dissociation rate coeffic	, ,
electronically excited diatomic gases	390 (2004) 370
Amoureux, J.P., see Ganapathy, S.	390 (2004) 79
Andrade, A.A., N.M. Barbosa Neto, L. Misoguti, L. De Boni, S.C. Zilio and C.R. Me	, ,
Two-photon absorption investigation in reduced and oxidized cytochrome c solutions Anestopoulos, D., G. Tsigaridas, P. Persephonis, V. Giannetas, I. Spiliopoulos, P. Kar and J. Mikroyannidis, Electro-optic characterization of two novel organic materials	390 (2004) 506 rastatiris
polymeric films	390 (2004) 98
Data Transcription In W	200 (2004) 25
Baba, T., see Shinoda, W.	390 (2004) 35
Baguenard, B., see Wills, J.B.	390 (2004) 145
Barbosa Neto, N.M., see Andrade, A.A.	390 (2004) 506
Bauschlicher Jr., C.W., A. Ricca, Y. Xue and M.A. Ratner, Current-voltage curves for m	
junctions: pyrene vs diphenylacetylene Proveni M. G. Pietranargia, F. Castellysei and Ph. Práchignas, Dynamics of vibranically	390 (2004) 246
Becucci, M., G. Pietraperzia, E. Castellucci and Ph. Bréchignac, Dynamics of vibronically states of the aniline–neon van der Waals complex: vibrational predissociation	
intramolecular vibrational redistribution	390 (2004) 29
Belytschko, T., see Mielke, S.L.	390 (2004) 413
Besley, N.A., Calculation of the electronic spectra of molecules in solution and on surfa	
Bettinelli, M., see Boyer, J.C.	390 (2004) 403
Beutter, M., see De Waele, V.	390 (2004) 328
Blanco, M., see Jacob, T.	390 (2004) 352
Blin, JL., see Gilles, F.	390 (2004) 236
Bondo Pedersen, T., see García Cuesta, I.	390 (2004) 170
Bordas, C., see Wills, J.B.	390 (2004) 145
Boskovic, C., see Schaniel, D.	390 (2004) 347
Boyer, J.C., F. Vetrone, J.A. Capobianco, A. Speghini and M. Bettinelli, Yb3+ ion as a s	
for the upconversion luminescence in nanocrystalline Gd ₃ Ga ₅ O ₁₂ :Ho ³⁺	390 (2004) 403
Bozon-Verduraz, F., see Izgaliev, A.T.	390 (2004) 467
Brady Moreira, F.G., see Marques Leite dos Santos, V.	390 (2004) 157
Bréchignac, Ph., see Becucci, M.	390 (2004) 29
Brutschy, B., see Wu, R.	390 (2004) 272
Bukalov, S.S., see Kononova, E.G.	390 (2004) 279
Burgers, P.C., see Wong, C.Y.	390 (2004) 176
Burghardt, B., see Merlitz, H.	390 (2004) 500
Burke, B.J., see Dailey, C.A.	390 (2004) 8

Capobianco, J.A., see Boyer, J.C.	390 (2004) 403
Car, R., see Mielke, S.L.	390 (2004) 413
Carravetta, M., see Kristiansen, P.E.	390 (2004) 1
Castellucci, E., see Becucci, M.	390 (2004) 29
Chan, WM., see Chan, MC.	390 (2004) 340
Chan, MC., SH. Yeung, YY. Wong, Y. Li, WM. Chan and KH. Yim, Near infrared	200 (2004) 240
absorptions of CH ₄ /He plasma: the Phillips band system of C ₂	390 (2004) 340
Chang, Y.J., see Park, S.J.	390 (2004) 199
Chatterjee, A., M. Nishioka and F. Mizukami, A periodic first principle study to design	200 (2004) 225
microporous crystal 12MO, 7Al ₂ O ₃ for selective and active O ⁻ radicals encaging	390 (2004) 335
Cheetham, A.K., see Gilles, F.	390 (2004) 236
Chen, P., see Zhao, P.D. Chen, Q., see Wang, J.	390 (2004) 41 390 (2004) 55
Chen, W.J., see Zhao, P.D.	390 (2004) 33
Chen, G., see Zheng, X.	390 (2004) 41
Cheung, E.Y., see Habershon, S.	390 (2004) 394
Chibisov, A.K., H. Görner and T.D. Slavnova, Kinetics of salt-induced J-aggregation of an	370 (2004) 374
anionic thiacarbocyanine dye in aqueous solution	390 (2004) 240
Chichinin, A.I., T.S. Einfeld, C. Maul and KH. Gericke, Photoionization of NO($A^2\Sigma^+$, $v=0,N$)	390 (2001) 240
at 226 nm: ion-recoil momentum spectroscopy	390 (2004) 50
Chikhaoui, A., see Aliat, A.	390 (2004) 370
Chizhevsky, I.T., see Kononova, E.G.	390 (2004) 279
Churikov, V.M., see Liu, S.	390 (2004) 433
Ciacchi, L.C. and M.C. Payne, The entry pathway of O2 into human ferritin	390 (2004) 491
Cogdell, R.J., see Rondonuwu, F.S.	390 (2004) 314
Cong, Y., see Li, J.	390 (2004) 285
Cyriac, J., V.R. Rajeev Kumar and T. Pradeep, Gas phase aggregates of protected clusters	390 (2004) 181
Dailey, C.A., B.J. Burke and G.J. Simpson, The general failure of Kleinman symmetry in practical	
nonlinear optical applications	390 (2004) 8
Daub, J., see De Waele, V.	390 (2004) 328
De Boni, L., see Andrade, A.A.	390 (2004) 506
De Waele, V., M. Beutter, U. Schmidhammer, E. Riedle and J. Daub, Switching dynamics of the	
photochromic 1,1-dicyano-2-(4-cyanophenyl)-1,8a-dihydroazulene probed by sub-30 fs spectro-	
scopy	390 (2004) 328
Denecke, R., see Fuhrmann, T.	390 (2004) 208
Deng, J.K., see Su, G.L.	390 (2004) 162
Díaz, C., see Farías, D.	390 (2004) 250
Ding, CG. and K. Laasonen, Partially and fully deprotonated sulfuric acid in $H_2SO_4(H_2O)_n$	200 (2004) 207
(n = 6-9) clusters	390 (2004) 307
Donovan, R.J., see Ridley, T.	390 (2004) 376
Downes, J.E., C. McGuinness, PA. Glans, T. Learmonth, D. Fu, P. Sheridan and K.E. Smith,	390 (2004) 203
Electronic structure near the Fermi level of the organic semiconductor copper phthalocyanine	390 (2004) 203
Dubois, V., P. Umari and A. Pasquarello, Dielectric susceptibility of dipolar molecular liquids by ab initio molecular dynamics: application to liquid HCl	390 (2004) 193
Dunne, L.J. and G. Manos, Exact statistical mechanical treatment of a toroidal lattice model of	390 (2004) 193
narrow-bore nanotube alkane adsorption isotherms and comparison with Monte-Carlo	
simulations	390 (2004) 14
Dzhagarov, B.M. and S.V. Lepeshkevich, Kinetic studies of differences between α - and β -chains of	370 (2004) 14
human hemoglobin: an approach for determination of the chain affinity to oxygen	390 (2004) 59
nominal nemogration an approach for determination of the chain animity to oxygen	(2001)
Eckern, U., see Eyert, V.	390 (2004) 151
Einfeld, T.S., see Chichinin, A.I.	390 (2004) 50
Endo, M., see Nishikiori, H.	390 (2004) 389
Eyert, V., U. Schwingenschlögl and U. Eckern, Charge order, orbital order, and electron	
localization in the Magnéli phase Ti ₄ O ₇	390 (2004) 151

Fan, W.Y., see Li, P.	390 (2004) 323
Farías, D., C. Díaz, P. Nieto, A. Salin and F. Martín, Pronounced out-of-plane diffraction of H ₂	200 (2004) 250
molecules from a Pd(1 1 1) surface	390 (2004) 250
Fernandez, C., see Ganapathy, S.	390 (2004) 79
Ferraro, M.B., P. Lazzeretti, R.G. Viglione and R. Zanasi, Understanding proton magnetic	200 (2004) 269
shielding in the benzene molecule	390 (2004) 268
Fritzsche, S., see Loisruangsin, A.	390 (2004) 485
Fu, D., see Downes, J.E. Fu, J., see Li, J.	390 (2004) 203 390 (2004) 285
Fuhrmann, T., M. Kinne, C.M. Whelan, J.F. Zhu, R. Denecke and HP. Steinrück, Vibrationally	390 (2004) 203
resolved in situ XPS study of activated adsorption of methane on Pt(111)	390 (2004) 208
Fujii, R., see Rondonuwu, F.S.	390 (2004) 314
Fujii, Y., see Ono, Y.	390 (2004) 71
Fujii, Y., see Ono, Y.	390 (2004) 421
Fujii, R., see Gloter, A.	390 (2004) 462
Fujii, T., see Nishikiori, H.	390 (2004) 389
rujii, 1., see ivisiirkioti, 11.	390 (2004) 309
Ganapathy, S., R. Kumar, V. Montouillout, C. Fernandez and J.P. Amoureux, Identification of tetrahedrally ordered Si-O-Al environments in molecular sieves by {27Al}-29Si REAPDOR NMR	300 (2004) 70
	390 (2004) 79 390 (2004) 296
Gao, X.D., see Yu, W.D.	390 (2004) 290
Gao, ZM., see Li, QS. García Cuesta, I., T. Bondo Pedersen, H. Koch and A.M.J. Sánchez de Merás, Polarizabilities of	390 (2004) 220
small annulenes from Cholesky CC2 linear response theory	390 (2004) 170
Garnache, A., see Gherman, T.	390 (2004) 170
Gericke, KH., see Chichinin, A.I.	390 (2004) 290
Gherman, T., D. Romanini, I. Sagnes, A. Garnache and Z. Zhang, Cavity-enhanced absorption	390 (2004) 30
spectroscopy with a mode-locked diode-pumped vertical external-cavity surface-emitting laser	390 (2004) 290
Giannetas, V., see Anestopoulos, D.	390 (2004) 290
Gilles, F., JL. Blin, C. Mellot-Draznieks, A.K. Cheetham and BL. Su, Neutron diffraction	390 (2004) 98
evidence of double interaction between NaY zeolite and ammonia and migration of Na ⁺ ions	
upon ND ₃ adsorption	390 (2004) 236
Glans, PA., see Downes, J.E.	390 (2004) 203
Gloter, A., K. Suenaga, H. Kataura, R. Fujii, T. Kodama, H. Nishikawa, I. Ikemoto, K. Kikuchi,	370 (2004) 203
S. Suzuki, Y. Achiba, and S. Iijima, Structural evolutions of carbon nano-peapods under	
electron microscopic observation	390 (2004) 462
Goddard III, W.A., see Jacob, T.	390 (2004) 352
Gong, LF., see Li, QS.	390 (2004) 220
Gordon, K.C., see Strachan, C.J.	390 (2004) 20
Görner, H., see Chibisov, A.K.	390 (2004) 240
Grasso, D., see Pappalardo, M.	390 (2004) 511
Güdel, HU., see Schaniel, D.	390 (2004) 347
Ha, J.S., see Park, S.J.	390 (2004) 199
Habershon, S., E.Y. Cheung, K.D.M. Harris and R.L. Johnston, An efficient algorithm for	
calculating whole-profile functions in crystal structure solution from powder diffraction data	390 (2004) 394
Hamilton, I.P., Complexes of cationic coinage metal clusters M_n^+ (M=Cu, Ag, Au; $n=1-4$) and	
H ₂ S: a theoretical study	390 (2004) 517
Han, Y., see Li, J.	390 (2004) 285
Hannongbua, S., see Loisruangsin, A.	390 (2004) 485
Harris, K.D.M., see Habershon, S.	390 (2004) 394
Hato, M., see Shinoda, W.	390 (2004) 35
Hirose, T., T. Omatsu, M. Sugiyama, S. Inasawa and S. Koda, Au-nano-particles production by	
pico-second ultra-violet laser deposition in Au-ion doped PMMA film	390 (2004) 166
Hobza, P., see Pittner, J.	390 (2004) 496
Hoyle, R.B., see Irurzun, I.M.	390 (2004) 305

Hsu, C.C., see Liu, S.	390 (2004) 433
Hsu, CP., see You, ZQ.	390 (2004) 116
Hu, L., see Zheng, X.	390 (2004) 186
Hu, H.Y. and E. Ruckenstein, Endohedral complexes of C ₅₈ cage with H ₂ and CO	390 (2004) 472
Huang, J.P., Force acting on the microparticles in electrorheological solids under the application	200 (2004) 200
of a nonuniform ac electric field	390 (2004) 380
Huang, J. and M. Kertesz, Intermolecular transfer integrals for organic molecular materials: can	200 (2004) 110
basis set convergence be achieved?	390 (2004) 110
Huang, F., see Su, G.L. Huang, TH., see Liu, S.	390 (2004) 162
Huang, 1H., see Liu, S.	390 (2004) 433
Iijima, S., see Gloter, A.	390 (2004) 462
Ikemoto, I., see Gloter, A.	390 (2004) 462
Ikezoe, Y., see Takahashi, M.	390 (2004) 104
Illenberger, E., see Abdoul-Carime, H.	390 (2004) 481
Inasawa, S., see Hirose, T.	390 (2004) 166
Inokuchi, Y., K. Ohshimo, F. Misaizu and N. Nishi, Structures of [Mg·(H ₂ O) _{1,2}] ⁺ and	230 (2001) 100
[Al·(H ₂ O) _{1,2}] ⁺ ions studied by infrared photodissociation spectroscopy: evidence of [HO-Al-	
H] ⁺ ion core structure in [Al·(H ₂ O) ₂] ⁺	390 (2004) 140
Irurzun, I.M., R.B. Hoyle, M.R.E. Proctor and D.A. King, Reply to 'Comment on 'Modelling	(
pattern formation in $CO + O_2$ on $Pt\{100\}$ "	390 (2004) 305
Ishida, T., see Ono, Y.	390 (2004) 421
Ishida, T., see Ono, Y.	390 (2004) 71
Ishigaki, T., see Miyagi, T.	390 (2004) 399
Izgaliev, A.T., A.V. Simakin, G.A. Shafeev and F. Bozon-Verduraz, Intermediate phase upon	250 (2001) 255
alloying Au-Ag nanoparticles under laser exposure of the mixture of individual colloids	390 (2004) 467
Jacob, T., M. Blanco and W.A. Goddard III, A new alligator-clip compound for molecular	200 (2004) 252
electronics	390 (2004) 352
Jensen, S.K., see Keiding, S.R.	390 (2004) 94
Johnston, R.L., see Habershon, S.	390 (2004) 394
Kamei, M., see Miyagi, T.	390 (2004) 399
Karastatiris, P., see Anestópoulos, D.	390 (2004) 399
Kataura, H., see Gloter, A.	390 (2004) 462
Keiding, S.R., D. Madsen, J. Larsen, S.K. Jensen and J. Thøgersen, When molecules meet: a	390 (2004) 402
femtosecond study of the protonation of a base	390 (2004) 94
Kertesz, M., see Huang, J.	390 (2004) 110
	390 (2004) 110
Khriachtchev, L., see Lignell, A.	390 (2004) 230
Kikuchi, K., see Gloter, A.	, ,
Kim, B., see Ahn, DS.	390 (2004) 384
Kim, G.T., see Park, S.J.	390 (2004) 199
King, D.A., see Irurzun, I.M.	390 (2004) 305
Kinne, M., see Fuhrmann, T.	390 (2004) 208
Kis, Z., see Thanopulos, I.	390 (2004) 228
Knospe, A.G. and A.S. Kwok, Spectral broadening in a microdroplet dye laser	390 (2004) 130
Koch, H., see García Cuesta, I.	390 (2004) 170
Koda, S., see Hirose, T.	390 (2004) 166
Kodama, T., see Gloter, A.	390 (2004) 462
Kononova, E.G., L.A. Leites, S.S. Bukalov, A.V. Zabula, I.V. Pisareva, V.E. Konoplev and I.T.	
Chizhevsky, Experimental and theoretical study of the vibrational spectrum, structure and	200 (2004) 270
electron density distribution of the [2-CB ₁₀ H ₁₁] ⁻ anion	390 (2004) 279
Konopley, V.E., see Kononova, E.G.	390 (2004) 279
Koyama, Y., see Rondonuwu, F.S.	390 (2004) 314
Kristiansen, P.E., M. Carravetta, W.C. Lai and M.H. Levitt, A robust pulse sequence for the	200 (2004)
determination of small homonuclear dipolar couplings in magic-angle spinning NMR	390 (2004) 1

Krstić, V., G. Wagnière and G.L.J.A. Rikken, Magneto-dynamics of chiral carbon nanotubes	390 (2004) 25	
Kubota, S., see Nishikiori, H.	390 (2004) 389	9
Kumar, R., see Ganapathy, S.	390 (2004) 79	
Kustova, E.V., see Aliat, A.	390 (2004) 370	0
Kwok, A.S., see Knospe, A.G.	390 (2004) 130	0
La Rosa, C., see Pappalardo, M.	390 (2004) 511	1
Laasonen, K., see Ding, CG.	390 (2004) 307	
Lai, W.C., see Kristiansen, P.E.	390 (2004)	
Larsen, J., see Keiding, S.R.	390 (2004) 94	
Lawley, K.P., see Ridley, T.	390 (2004) 376	
Lazzeretti, P., see Ferraro, M.B.	390 (2004) 268	
Learmonth, T., see Downes, J.E.	390 (2004) 203	
Lee, S., see Ahn, DS.	390 (2004) 384	
Leites, L.A., see Kononova, E.G.	390 (2004) 279	
Lepeshkevich, S.V., see Dzhagarov, B.M.	390 (2004) 59	
Lépine, F., see Wills, J.B.	390 (2004) 145	
Levitt, M.H., see Kristiansen, P.E.	390 (2004) 14.	
Li, JL., see Mielke, S.L.	390 (2004) 413	
	, ,	
Li, Y., see Chan, MC.	390 (2004) 340	
Li, QS., LF. Gong and ZM. Gao, Structures and stabilities of B_7 , B_7^+ and B_7^- clusters	390 (2004) 220	
Li, B., see Su, G.L.	390 (2004) 162	
Li, P. and W.Y. Fan, Energy distributions of CO produced in an acetone-containing discharge	390 (2004) 323	3
Li, J., Y. Wu, J. Fu, Y. Cong, J. Peng and Y. Han, Reversibly strain-tunable elastomeric photonic	200 (2004) 20	-
crystals	390 (2004) 28:	
Li, G.Q., see Su, G.L.	390 (2004) 162	
Li, X., see Wang, J.	390 (2004) 5:	
Li, X.M., see Yu, W.D.	390 (2004) 290	
Li, C., see Zhang, B.	390 (2004) 63	5
Lignell, A., L. Khriachtchev, M. Räsänen and M. Pettersson, A study on stabilization of HHeF		
molecule upon complexation with Xe atoms	390 (2004) 250	
Lin, J.L., see Zhang, B.	390 (2004) 6	
Lin, J.T., see Liu, S.	390 (2004) 43:	
Lin, K.S., see Liu, S.	390 (2004) 43:	
Liu, P., see Meier, J.	390 (2004) 440	0
Liu, S., K.S. Lin, V.M. Churikov, Y.Z. Su, J.T. Lin, TH. Huang and C.C. Hsu, Two-photon		
absorption properties of star-shaped molecules containing peripheral diarylthienylamines	390 (2004) 43	3
Loisruangsin, A., S. Fritzsche and S. Hannongbua, Newly developed ab initio fitted potentials for		
molecular dynamics simulations of <i>n</i> -pentane in the zeolite silicalite-1	390 (2004) 48	
Longo, R.L., see Marques Leite dos Santos, V.	390 (2004) 15	7
Madsen, D., see Keiding, S.R.	390 (2004) 9)4
Manos, G., see Dunne, L.J.	390 (2004) 1	
Marques Leite dos Santos, V., F.G. Brady Moreira and R.L. Longo, Topology of the hydrogen	370 (2004)	7
bond networks in liquid water at room and supercritical conditions: a small-world structure	390 (2004) 15	57
Martín, F., see Farías, D.	390 (2004) 15	
Maul, C., see Chichinin, A.I.	390 (2004) 25	
Maximoff, S.N. and G.E. Scuseria, Nuclear magnetic resonance shielding tensors calculated with	390 (2004) 3	,0
kinetic energy density-dependent exchange-correlation functionals	390 (2004) 40	10
McGuinness, C., see Downes, J.E.	, ,	
	390 (2004) 20	
Meier, J., J. Schiøtz, P. Liu, J.K. Nørskov and U. Stimming, Nano-scale effects in electrochemistry	390 (2004) 44	
Mellot-Draznieks, C., see Gilles, F. Mendonça, C.R., see Andrade, A.A.	390 (2004) 23	
Meng, L., see Zeng, Y.	390 (2004) 50	
Michel, L., See Zeng, 1.	200 (2004) 26	3
Marlitz H. R. Rurghardt and W. Wanzal Impact of recentor conformation on in cities accoming	390 (2004) 36	52
Merlitz, H., B. Burghardt and W. Wenzel, Impact of receptor conformation on in silico screening performance	390 (2004) 36 390 (2004) 50	

Mielke, S.L., D. Troya, S. Zhang, JL. Li, S. Xiao, R. Car, R.S. Ruoff, G.C. Schatz and	
T. Belytschko, The role of vacancy defects and holes in the fracture of carbon nanotubes	390 (2004) 413
Mikami, M., see Shinoda, W.	390 (2004) 35
Mikroyannidis, J., see Anestopoulos, D.	390 (2004) 98
Milardi, D., see Pappalardo, M.	390 (2004) 511
Mimuro, M., see Akimoto, S.	390 (2004) 45
Misaizu, F., see Inokuchi, Y.	390 (2004) 140
Misoguti, L., see Andrade, A.A.	390 (2004) 506
Mitsuhashi, T., see Miyagi, T.	390 (2004) 399
Miyagi, T., M. Kamei, T. Mitsuhashi, T. Ishigaki and A. Yamazaki, Charge separation at the	370 (2001) 377
rutile/anatase interface: a dominant factor of photocatalytic activity	390 (2004) 399
Mizukami, F., see Chatterjee, A.	390 (2004) 335
Mohapatra, H. and S. Umapathy, Time resolved resonance Raman studies on triplet excited state	270 (2001) 222
of 2-methoxy-naphthalene by photo-sensitization	390 (2004) 427
Montouillout, V., see Ganapathy, S.	390 (2004) 79
Muga, J.G. and B. Navarro, Comparison between semiclassical and composite absorbing	370 (2004) 17
potentials	390 (2004) 454
Murakami, A., see Akimoto, S.	390 (2004) 45
Tratakami, 71., see 71kmoto, 5.	370 (2004) 43
Nagase, S., see Ono, Y.	390 (2004) 71
Napolitano, R.d.J., see Ribeiro, E.M.S.	390 (2004) 89
Navarro, B., see Muga, J.G.	390 (2004) 454
Newnham, D.A., see Strachan, C.J.	390 (2004) 20
Nieto, P., see Farías, D.	390 (2004) 250
Ning, C.G., see Su, G.L.	390 (2004) 162
Nishi, N., see Inokuchi, Y.	390 (2004) 140
Nishikawa, H., see Gloter, A.	390 (2004) 462
Nishikiori, H., N. Tanaka, S. Kubota, M. Endo and T. Fujii, In situ characterization of surface	270 (2001) 102
physicochemical properties of carbon nanofibers using 1-naphthol as a fluorescent probe	390 (2004) 389
Nishioka, M., see Chatterjee, A.	390 (2004) 335
Nørskov, J.K., see Meier, J.	390 (2004) 440
	(200.)
Ohshimo, K., see Inokuchi, Y.	390 (2004) 140
Ohtawara, K. and H. Teramae, Study on optimization of molecular structure using Hamiltonian	(
algorithm	390 (2004) 84
Omatsu, T., see Hirose, T.	390 (2004) 166
Ono, Y., Y. Fujii, S. Nagase and T. Ishida, A density functional theory study applied for carbon	(,
isotope effects in the non-aqueous [Cu(CO)] ⁺ /CO system	390 (2004) 71
Ono, Y., Y. Fujii and T. Ishida, A density functional theory study applied for carbon and oxygen	()
isotope effects in the system Ni(CO) ₄ /CO	390 (2004) 421
Orwa, J.O., see Prawer, S.	390 (2004) 458
Ovadia, M. and D.H. Zavitz, Impedance spectroscopy of the electrode-tissue interface of living	()
heart with isoösmotic conductivity perturbation	390 (2004) 445
The state of the s	()
Pagliarulo, F., see Wills, J.B.	390 (2004) 145
Pappalardo, M., D. Milardi, C. La Rosa, C. Zannoni, E. Rizzarelli and D. Grasso, A molecular	
dynamics study on the conformational stability of PrP 180–193 helix II prion fragment	390 (2004) 511
Park, S.J., J.S. Ha, Y.J. Chang and G.T. Kim, Time dependent evolution of vanadium pentoxide	()
nanowires in sols	390 (2004) 199
Paspalakis, E., see Thanopulos, I.	390 (2004) 228
Pasquarello, A., see Dubois, V.	390 (2004) 193
Payne, M.C., see Ciacchi, L.C.	390 (2004) 491
Peng, J., see Li, J.	390 (2004) 285
Peng, Z., see Wang, J.	390 (2004) 55
Pepper, M., see Strachan, C.J.	390 (2004) 20
Persephonis, P., see Anestopoulos, D.	390 (2004) 98
Total Production of the state o	(===,)

Pettersson, M., see Lignell, A.	390 (2004) 256
Pichierri, F., Density functional study of cucurbituril and its sulfur analogue	390 (2004) 214
Pietraperzia, G., see Becucci, M.	390 (2004) 29
Pisareva, I.V., see Kononova, E.G.	390 (2004) 279
Pittner, J. and P. Hobza, CCSDT and CCSD(T) calculations on model H-bonded and stacked	
complexes	390 (2004) 496
Pradeep, T., see Cyriac, J.	390 (2004) 181
Prasad, M.A. and M.V. Sangaranarayanan, Solvent effect on the electrochemical reductive	
cleavage of carbon tetrachloride - a novel example of the deviation from the quadratic	
activation-driving force relationship	390 (2004) 261
Prawer, S., I. Rosenblum, J.O. Orwa and J. Adler, Identification of the point defects in diamond as	
measured by Raman spectroscopy: comparison between experiment and computation	390 (2004) 458
Proctor, M.R.E., see Irurzun, I.M.	390 (2004) 305
Rades, T., see Strachan, C.J.	390 (2004) 20
Rajeev Kumar, V.R., see Cyriac, J.	390 (2004) 181
Räsänen, M., see Lignell, A.	390 (2004) 256
Ratner, M.A., see Bauschlicher Jr., C.W.	390 (2004) 246
Ren, X.G., see Su, G.L.	390 (2004) 162
Ribeiro, E.M.S., A.L.M. Zanelatto and R.d.J. Napolitano, High-intensity and ground-state	
influence on photoassociation line shapes of ⁸⁸ Sr	390 (2004) 89
Ribeiro-Claro, P.J.A. and P.D. Vaz, Towards the understanding of the spectroscopic behaviour of	
the C-H oscillator in C-HO hydrogen bonds: the effect of solvent polarity	390 (2004) 358
Ricca, A., see Bauschlicher Jr., C.W.	390 (2004) 246
Ridley, T., K.P. Lawley, M.H.S.N. Al-Kahali and R.J. Donovan, Determination of the first	, , , ,
ionization energy of furan (C ₄ H ₄ O) from an extrapolation of two nd Rydberg series observed in	
the mass-resolved (2 + 1) resonance enhanced multiphoton ionization spectrum	390 (2004) 376
Riedle, E., see De Waele, V.	390 (2004) 328
Rikken, G.L.J.A., see Krstić, V.	390 (2004) 25
Rizzarelli, E., see Pappalardo, M.	390 (2004) 511
Romanini, D., see Gherman, T.	390 (2004) 290
Rondonuwu, F.S., K. Yokoyama, R. Fujii, Y. Koyama, R.J. Cogdell and Y. Watanabe, The role	
of the 1 ¹ B _u state in carotenoid-to-bacteriochlorophyll singlet-energy transfer in the LH2	
antenna complexes from Rhodobacter sphaeroides G1C, Rhodobacter sphaeroides 2.4.1,	
Rhodospirillum molischianum and Rhodopseudomonas acidophila	390 (2004) 314
Rosenblum, I., see Prawer, S.	390 (2004) 458
Ruckenstein, E., see Hu, H.Y.	390 (2004) 472
Ruoff, R.S., see Mielke, S.L.	390 (2004) 413
Ruttink, P.J.A., see Wong, C.Y.	390 (2004) 176
Salin, A., see Farías, D.	390 (2004) 250
Sagnes, I., see Gherman, T.	390 (2004) 290
Sánchez de Merás, A.M.J., see García Cuesta, I.	390 (2004) 170
Sangaranarayanan, M.V., see Prasad, M.A.	390 (2004) 261
Sawada, T., see Takahashi, M.	390 (2004) 104
Schaniel, D., T. Woike, C. Boskovic and HU. Güdel, Evidence for two light-induced metastable	
states in Cl ₃ [Ru(NH ₃) ₅ NO]H ₂ O	390 (2004) 347
Schatz, G.C., see Mielke, S.L.	390 (2004) 413
Schiøtz, J., see Meier, J.	390 (2004) 440
Schmidhammer, U., see De Waele, V.	390 (2004) 328
Schwingenschlögl, U., see Eyert, V.	390 (2004) 151
Scuseria, G.E., see Maximoff, S.N.	390 (2004) 408
Shafeev, G.A., see Izgaliev, A.T.	390 (2004) 467
Shao, Y., see You, ZQ.	390 (2004) 116
Sheridan, P., see Downes, J.E.	390 (2004) 203
Shi, L., see Wang, J.	390 (2004) 55

Shinoda, W., M. Mikami, T. Baba and M. Hato, Dynamics of a highly branched lipid bilayer: a	
molecular dynamics study	390 (2004) 35
Simakin, A.V., see Izgaliev, A.T.	390 (2004) 467
Simpson, G.J., see Dailey, C.A.	390 (2004) 8
Slavnova, T.D., see Chibisov, A.K.	390 (2004) 240
Smith, K.E., see Downes, J.E.	390 (2004) 203
Speghini, A., see Boyer, J.C.	390 (2004) 403
Spiliopoulos, I., see Anestopoulos, D.	390 (2004) 98
Steinrück, HP., see Fuhrmann, T.	390 (2004) 208
Stimming, U., see Meier, J.	390 (2004) 440
Strachan, C.J., T. Rades, D.A. Newnham, K.C. Gordon, M. Pepper and P.F. Taday, Using	
terahertz pulsed spectroscopy to study crystallinity of pharmaceutical materials	390 (2004) 20
Su, Y.Z., see Liu, S.	390 (2004) 433
Su, G.L., C.G. Ning, S.F. Zhang, X.G. Ren, H. Zhou, B. Li, F. Huang, G.Q. Li, J.K. Deng and Y. Wang, An electron momentum spectroscopy study of the highest occupied molecular orbital of	
difluoromethane	390 (2004) 162
Su, H., see Zhang, B.	390 (2004) 65
Su, BL., see Gilles, F.	390 (2004) 236
Suenaga, K., see Gloter, A.	390 (2004) 462
Sugiyama, M., see Hirose, T.	390 (2004) 166
Sun, Q., see Zeng, Y.	390 (2004) 362
Suzuki, S., see Gloter, A.	390 (2004) 462
Tachiya, M., see Wojcik, M.	390 (2004) 475
Taday, P.F., see Strachan, C.J.	390 (2004) 20
Tahara, T., see Yamaguchi, S.	390 (2004) 136
Takahashi, M., H. Yui, Y. Ikezoe and T. Sawada, Anomalous change in interfacial tension	
induced by collapses of AOT microemulsions at heptane/water interface	390 (2004) 104
Takaichi, S., see Akimoto, S.	390 (2004) 45
Tanaka, N., see Nishikiori, H.	390 (2004) 389
Tang, G.Q., see Zhao, P.D.	390 (2004) 41 390 (2004) 84
Teramae, H., see Ohtawara, K. Terlouw, J.K., see Wong, C.Y.	390 (2004) 176
Thøgersen, J., see Keiding, S.R.	390 (2004) 170
Thanopulos, I., E. Paspalakis and Z. Kis, Laser-driven coherent manipulation of molecular	370 (2004) 74
chirality	390 (2004) 228
Troya, D., see Mielke, S.L.	390 (2004) 413
Tsigaridas, G., see Anestopoulos, D.	390 (2004) 98
Tzeng, W.B., see Zhang, B.	390 (2004) 65
Umapathy, S., see Mohapatra, H.	390 (2004) 427
Umari, P., see Dubois, V.	390 (2004) 193
Vaz, P.D., see Ribeiro-Claro, P.J.A.	390 (2004) 358
Vetrone, F., see Boyer, J.C.	390 (2004) 403
Viglione, R.G., see Ferraro, M.B.	390 (2004) 268
Wagnière, G., see Krstić, V.	390 (2004) 25
Wang, J., Q. Chen, X. Li, L. Shi, Z. Peng and C. Zeng, Disappearing of the Verwey transition in magnetite nanoparticles synthesized under a magnetic field: implications for the origin of charge	
ordering	390 (2004) 55
Wang, X., see Zheng, X.	390 (2004) 186
Wang, D., see Zeng, Y.	390 (2004) 362
Wang, Y., see Su, G.L.	390 (2004) 162
Watanabe, Y., see Rondonuwu, F.S.	390 (2004) 314
Wenzel, W., see Merlitz, H.	390 (2004) 500

Whelan, C.M., see Fuhrmann, T.	390 (2004) 208
Wills, J.B., F. Pagliarulo, B. Baguenard, F. Lépine and C. Bordas, Time and kinetic energy	
resolved delayed electron emission in small carbon cluster anions	390 (2004) 145
Woike, T., see Schaniel, D.	390 (2004) 347
Wojcik, M. and M. Tachiya, Electron-ion recombination in dense gaseous and liquid argon: effects	
due to argon cation clusters allow to explain the experimental data	390 (2004) 475
Wong, YY., see Chan, MC.	390 (2004) 340
Wong, C.Y., P.J.A. Ruttink, P.C. Burgers and J.K. Terlouw, The isomerization of [H ₂ O-C=O] ⁺	
and [HC(=O)OH] ⁺⁺ into [HO-C-OH] ⁺⁺ : proton-transport catalysis by CO	390 (2004) 176
Wu, Y., see Li, J.	390 (2004) 285
Wu, R. and B. Brutschy, Study on the structure and intra- and intermolecular hydrogen bonding	
of 2-methoxyphenol \cdot (H ₂ O) _n (n = 1, 2)	390 (2004) 272
Xiao, S., see Mielke, S.L.	390 (2004) 413
Xue, Y., see Bauschlicher Jr., C.W.	390 (2004) 246
Yamaguchi, S. and T. Tahara, Observation of an optically forbidden state of C ₆₀ by	
nondegenerate two-photon absorption spectroscopy	390 (2004) 136
Yamazaki, I., see Akimoto, S.	390 (2004) 45
Yamazaki, A., see Miyagi, T.	390 (2004) 399
Yeung, SH., see Chan, MC.	390 (2004) 340
Yim, KH., see Chan, MC.	390 (2004) 340
Yokoyama, K., see Rondonuwu, F.S.	390 (2004) 314
You, ZQ., Y. Shao and CP. Hsu, Calculating electron transfer couplings by the Spin-Flip	()
approach: energy splitting and dynamical correlation effects	390 (2004) 116
Yu, W.D., X.M. Li and X.D. Gao, Homogeneous-catalytic synthesis of tetrapodlike ZnO	(,
nanocrystals and their photoluminescence properties	390 (2004) 296
Yui, H., see Takahashi, M.	390 (2004) 104
Zabula, A.V., see Kononova, E.G.	390 (2004) 279
Zanasi, R., see Ferraro, M.B.	390 (2004) 268
Zanelatto, A.L.M., see Ribeiro, E.M.S.	390 (2004) 89
Zannoni, C., see Pappalardo, M.	390 (2004) 511
Zavitz, D.H., see Ovadia, M.	390 (2004) 445
Zeng, Y., Q. Sun, L. Meng, S. Zheng and D. Wang, Theoretical calculational studies on the	
mechanism of thermal dissociations for RN ₃ (R=CH ₃ , CH ₃ CH ₂ , (CH ₃) ₂ CH, (CH ₃) ₃ C)	390 (2004) 362
Zeng, C., see Wang, J.	390 (2004) 55
Zhang, S.F., see Su, G.L.	390 (2004) 162
Zhang, S., see Mielke, S.L.	390 (2004) 413
Zhang, G.L., see Zhao, P.D.	390 (2004) 41
Zhang, Z., see Gherman, T.	390 (2004) 290
Zhang, B., C. Li, H. Su, J.L. Lin and W.B. Tzeng, Mass analyzed threshold ionization	
spectroscopy of p-fluorophenol cation and the p-fluoro substitution effect	390 (2004) 65
Zhao, P.D., P. Chen, G.Q. Tang, G.L. Zhang and W.J. Chen, Two-photon spectroscopic	()
properties of a new chlorin derivative photosensitizer	390 (2004) 41
Zhdanov, V.P., Comment on 'Modelling pattern formation in CO + O ₂ (reaction) on Pt{100}'	390 (2004) 301
Zheng, X., L. Hu, X. Wang and G. Chen, A generalized exchange-correlation functional: the	(400.)
Neural-Networks approach	390 (2004) 186
Zheng, S., see Zeng, Y.	390 (2004) 362
Zhou, H., see Su, G.L.	390 (2004) 162
Zhu, J.F., see Fuhrmann, T.	390 (2004) 208
Zilio, S.C., see Andrade, A.A.	390 (2004) 506
Zino, o.e., overmonde, rink	370 (2004) 300